

1,4-Dioxane
123-91-1 | DTXSID4020533

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 1.06

Global applicability domain: Inside

Local applicability domain index: 7.94e-01

Confidence level: 6.43e-01

Nearest Neighbors from the Training Set

Image not found

1,4-Dioxane

Measured: 5.01e-01

Predicted: 1.06

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N,N-Dimethylformamide

Measured: 7.94e-01

Predicted: 1.12

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Morpholine

Measured: 2.82

Predicted: 1.87

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Piperazine

Measured: 3.89

Predicted: 2.44

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4-Methylimidazolidine-2-thione

Measured: 10.0

Predicted: 4.59